Restoring fluctuation-dissipation relations in non equilibrium steady states

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Structure of the talk

1. Correlation-response relations in steady states

2. Two temperatures brownian motion (exactly solvable model)

3. Numerical analysis of response on granular gas models
Classical fluctuation-dissipation relations

**Einstein relation**

\[
\frac{\delta A(t)}{\delta h(0)} = \text{const.} \langle A(t)A(0) \rangle
\]

Valid for a Brownian particle in a fluid at temperature T

Equivalent to the integrated version

\[
\mu = \beta D
\]

Mobility (integrated response) \hspace{1cm} \text{Diffusion coefficient (integrated correlation)}

**Kubo relation**

\[
\frac{\delta A(t)}{\delta h(0)} = -\beta \frac{d}{dt} \langle A(t)B(0) \rangle
\]

Valid for Hamiltonian systems at temperature \( T = 1/\beta \) with a variation \( \delta \mathcal{H} = -\delta h(0)\delta(t)B \)

It also holds for a Langevin equation with a gradient structure

\[
\dot{x}_i = -\frac{1}{\gamma} \frac{\partial H}{\partial x_i} + \sqrt{2T/\gamma} \eta_i
\]
Generalized Fluctuation-dissipation relation (GFDR)


\[ \mathbf{x}(t) = S^t \mathbf{x}(0) \quad \text{Perturbed trajectory:} \quad \mathbf{x}'(0) = \mathbf{x}(0) + \delta \mathbf{x} \]

\[ \delta \mathbf{x} = (0, \ldots, \delta x_j, \ldots, 0) \]

Evolution operator

if \( \rho(\mathbf{x}) \) is a non vanishing and differentiable phase space distribution function and the system is mixing

Relaxation of an external perturbation

Steady state correlation (unperturbed system)

\[ \frac{\delta x_i(t)}{\delta x_j(0)} = - \left< x_i(t) \frac{\partial \ln \{ \rho(\mathbf{x}) \}}{\partial x_j} \right|_{t=0} \]

GFDR \( \rightarrow \quad \rho(\mathbf{x}) \propto e^{-\beta \phi(\mathbf{x})} \quad \text{Einstein relation} \quad \text{if} \quad \phi(\mathbf{x}) \quad \text{is quadratic} \)

Kubo relation \( \quad \text{if} \quad \phi(\mathbf{x}) = \mathcal{H}(\mathbf{x}) \)
2. Two temperatures brownian motion (exactly solvable model)
Brownian motion with memory: two thermostats case

\[ m \ddot{x} = -kx - \int_{-\infty}^{t} \gamma(t - t') \dot{x}(t') dt' + \rho_f(t) + \rho_s(t) \]

- Harmonic force
- Memory term
- \( \eta(t) \) Stochastic part

\[ \langle \rho_f(t) \rho_f(t') \rangle = 2 \gamma_f T_F \delta(t - t') \]
Fast thermostat (white noise)

\[ \langle \rho_s(t) \rho_s(t') \rangle = \frac{\gamma_s T_s}{\tau_s} e^{-\frac{|t-t'|}{\tau_s}} \]
Slow thermostat (red noise)

\[ \gamma(t) = 2 \gamma_f \delta(t) + \frac{\gamma_s}{\tau_s} e^{-\frac{t}{\tau_s}} \]
Brownian motion with memory: Equilibrium case \( (T_f = T_s) \)

Equilibrium case: \( T_f = T_s \) and \( \langle \eta(t) \eta(t') \rangle = T \gamma(t - t') \)

Free particle case: \( k = 0 \)

\[
R_{vv}(t) = C_{vv}(t)
\]

Overdamped regime

\[
R_{xx}(t) = -\beta \frac{d}{dt} \langle x(t) x(0) \rangle
\]

\[
\chi_{xx}(t) \equiv \int_0^t R_{xx}(t')dt' = \text{const} - \beta \langle x(t) x(0) \rangle
\]
Brownian motion with memory: two thermostats case ($T_f \neq T_s$)


Distribution of velocity $P(v)$ is always a gaussian with variance $T_{\text{eff}}$:

$$\min\{T_f, T_s\} < T_{\text{eff}} < \max\{T_f, T_s\}$$

Is this a violation of GFDR?
Memory as a hidden variable

\[ m\ddot{x} = -kx - \int_{-\infty}^{t} \gamma(t-t')x(t')dt' + \rho_f(t) + \rho_s(t) \]

Mapped in a two variables system

\[
\begin{pmatrix}
\dot{v} \\
\dot{u}
\end{pmatrix} = -\begin{pmatrix}
\gamma_f & -1 \\
\gamma_s & -1/	au_s
\end{pmatrix} \begin{pmatrix}
v \\
u
\end{pmatrix} + \begin{pmatrix}
\eta_1 \\
\eta_2
\end{pmatrix}
\]

Colored noise and memory term are not present
Memory as a hidden variable

How do you know you have taken enough variables, for it to be markovian?

Lars Onsager

Memory is a degree of freedom \( \implies \) Two variables Langevin equation

\[
\begin{pmatrix}
\dot{v} \\
\dot{u}
\end{pmatrix}
= - \begin{pmatrix}
\gamma_f & -\frac{1}{\tau_s} \\
\frac{\gamma_s}{\tau_s} & \frac{1}{\tau_s}
\end{pmatrix}
\begin{pmatrix}
v \\
u
\end{pmatrix}
+ \begin{pmatrix}
\eta_1 \\
\eta_2
\end{pmatrix}
\]

\( \rho(u,v) \) has a bivariate Gaussian shape:

\[
\ln \rho(u,v) = \sigma_{vv}^{-1} v^2 + \sigma_{uu}^{-1} u^2 + 2\sigma_{uv}^{-1} uv + \text{const}
\]

Application of GFDR

\[
R_{vv}(t) = - \left. \left\langle v(t) \frac{\partial \ln \rho(u,v)}{\partial v} \right\rangle \right|_{t=0}
\]

\[
R_{vv}(t) = \sigma_{vv}^{-1} \langle v(t) v(0) \rangle + \sigma_{uv}^{-1} \langle v(t) u(0) \rangle \neq C_{vv}
\]

\( \{ C_{vv}, C_{vu} \} \)

\( P(v) \) observed is a marginal distribution

\[
P(v) = \int \rho(u,v) du
\]
Considering the “missing” variable linearity is restored

$$\sigma_{uv} \propto (T_s - T_f)$$

Coupling effect vanishes at equilibrium

Similar considerations are also valid:

- in the overdamped regime
- when several thermostat are present

**Non linear relations** between $C_{vv}(t)$ and $R_{vv}(t)$ are due to the cross correlation term

**This is not a violation of generalized FDR!**
3. Numerical analysis of response on granular gas models
Granular gas model:
Puglisi, Baldassarri, Loreto - Physical Review E, 2002

\[
\frac{dx_i(t)}{dt} = v_i(t)
\]

\[
\frac{dv_i(t)}{dt} = -\frac{v_i(t)}{\tau_b} + \sqrt{\frac{2T_b}{\tau_b}} \eta_i(t)
\]

\[
\begin{align*}
\nu'_1 &= \nu_1 - \frac{1+r}{2}(\nu_1 - \nu_2) \\
\nu'_2 &= \nu_2 + \frac{1+r}{2}(\nu_1 - \nu_2)
\end{align*}
\]

Two times scale system

Mean collision time \( \tau_c \)

Thermostat time \( \tau_b \)

Equilibrium-like regime \( \tau_c >> \tau_b \)

Homogeneous spatial distribution
Maxwell distribution of velocities

\[
T_b = T_c
\]

Colliding regime \( \tau_c < \tau_b \)

Spatial inhomogeneity is present
Non-Maxwellian deviations can occur

\[
T_g \leq T_b
\]
Dilute regime:

Perturbation $\delta v_i(0)$ of tracer's velocity
(linear response regime)

$$\frac{\delta v_i(t)}{\delta v_i(0)} = - \left. \left< \frac{\partial \ln \rho \{x, v\}}{\partial v_i} \right|_{t=0} \right>$$

$$\rho \{x, v\} = n^N \prod_{i=1}^{N} p_v(v_i)$$

$$\frac{\delta v_i(t)}{\delta v_i(0)} = - \left. \left< v_i(t) \frac{\partial \ln p_v(v_i)}{\partial v_i} \right|_{t=0} \right>$$

Pdf is well fitted by

$$p_v(v) \approx c_0 \exp \left[ - \left( c_1 v^2 + c_2 |v^3| \right) \right]$$

One may expect

$$R(t) = -2c_1 \langle v(t)v(0) \rangle + 3c_2 \langle v(t)|v(0)|v(0) \rangle$$

Surprisingly

$$\langle v(t)v(0) \rangle \propto \langle v(t)|v(0)|v(0) \rangle$$

(very small deviations are observed)

**Einstein relation**

$$\frac{\delta v(t)}{\delta v(0)} = \frac{1}{T_g} \langle v(t)v(0) \rangle$$

**Granular Temperature** $T_g \leq T_b$

**Response**

**Autocorrelation**
Strong dissipation

Spatial inhomogeneity

\[ \rho(\{x, v\}) \neq n^N \prod_{i=1}^{N} p_v(v_i) \]

Coupling between different degrees of freedom produces non linear relations between \( C(t) \) and \( R(t) \)

\[ \alpha = \frac{\tau_c}{\tau_b} \]

Single particle factorization fails

\[ \frac{\delta v_i(t)}{\delta v_i(0)} \neq - \left\langle v_i(t) \frac{\partial \ln p_v(v_i)}{\partial v_i} \right|_{t=0} \right\rangle \]

In a strong dissipation regime, Einstein relation is not recovered

This is **not** a violation of Fluctuation-dissipation Relations (FDR)

**Generalized FDR**

\[ \frac{\delta v_i(t)}{\delta v_i(0)} = - \left\langle v_i(t) \frac{\partial \ln \rho(\{x, v\})}{\partial v_i} \right|_{t=0} \right\rangle \]
Restoring equilibrium-like relations

Simple ansatz on $\rho(\{x, v\})$ introducing a local velocity average field $u(x)$

$u(x)$ is defined on a small cell of diameter $L_{box}$ centered in the tracer

$$p_v(v, x, t) \sim \exp \left\{ -\frac{[v - u(x, t)]^2}{2T_g} \right\}$$

$$R(t) = C_s = \frac{1}{T_g} \langle v(t) \{v(0) - u[x(0)] \} \rangle$$

The generalized FDR can be used to verify hypothesis on the phase space distribution function.
A pedagogical mistake

Elastic regime

\[ R = C \]

\[ R \not\propto \dot{C} \]

Strong inelastic regime

\[ R \neq C \]

\[ R \propto \dot{C} \]

A misleading analysis of RC plot could cause paradoxes
(Two effective temperatures in the elastic case!)

Actually it is an effect of the non-trivial velocity correlation’s shape
Conclusions

In non equilibrium steady states, classical fluctuation-dissipation relations are non expected to hold.

It is possible to define a generalized formula relating response function to a correlation computed in the steady state.

A non linear relation between autocorrelation and response functions is due to couplings between different degrees of freedom.

The generalized relation can be used to verify onsets on the steady state distribution function.
Recent works on generalized fluctuation dissipation relation:

D. Villamaina, A. Baldassarri, A. Puglisi, A. Vulpiani, to be published

Paper we published on GFDR in granular gas models:

Numerical recipes for FDR computation

- The gas is left evolve from an initial condition until a statistically stationary state is reached.

- A copy of the system is obtained, identical to the original except one particle, whose velocity’s component is augmented of $\delta v_i(0)$.

- Both the systems are left evolve with the unperturbed dynamic (same noise is used).

Simulation are performed in a linear response regime

$\delta v(0) \ll \langle |v| \rangle \sim \sqrt{T_g}$